# ID Card
# Tetraamminepalladium(2+) diacetate

*Version 16 June 2016*

*Notes:*

- *This ID card is used to support the substance sameness discussions in SIEFs and to describe the substance to the best of the SIEF members' knowledge.*
- *It also aims at grouping communications relevant to the request of available data or information, the approval of the proposed Lead Registrant and the registration strategy with the SIEF.*
- *It is the responsibility of each individual registrant to identify their substance and to report company-specific identity in their Registration Dossier (section 1 of IUCLID).*



## 1. Identification of the substance

**Table 1. Identification of the substance**

| | Original (in EC inventory) |
|---|---|
| **Name** | Tetraamminepalladium(2+) diacetate |
| **EC number** | 262-819-1 |
| **CAS number** | 61495-96-3 |
| **Description** | Not available |
| **Composition type** | Mono-constituent substance |

## 2. Synonyms and other identifiers of the substance

**Table 2. Synonyms and other identifiers of the substance**

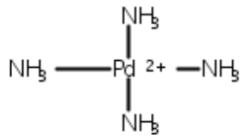
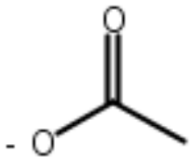
| | |
|---|---|
| **IUPAC name** | azane;palladium(2+);diacetate |
| **CAS name** | Palladium(2+), tetraammine-, (SP-4-1)-, acetate (1:2) |
| **Abbreviations** | |
| **Other commercial, brand or international names** | Palladium tetraammine diacetate<br>Tetraamminepalladium(II) acetate |
| **Other identity codes** | |

## 3. Substances (with core identifiers) also falling under this substance (with justification)

None

## 4. Information related to molecular and structural formula of the substance

**Table 3. Information related to molecular and structural formula of the substance**

| | |
|---|---|
| **Molecular formula** | C4H18N4O4Pd |
| **Structural formula** | 15974-14-8<br>$H_{12}N_4Pd$<br>  <br>71-50-1<br>$C_2H_3O_2$<br>  |
| **Smiles notation** | [Pd+2].[O-]C(=O)C.[O-]C(=O)C.N.N.N.N |
| **Optical activity** | Not applicable |
| **Typical ratio of (stereo) isomers** | Not applicable |
| **Molecular Weight / Molecular Weight range** | 292,63 g/mol |

## 5. Typical composition of the substance

**Table 4. Typical composition solid**

| | Name | Symbol / Formula | Min & Max concentrations (%)[§] | Typical concentration (%)[§§] |
|---|---|---|---|---|
| **Main constituent(s)*** | Tetraamminepalladium(2+) diacetate | C4H18N4O4Pd | 82 - 100[$] | 91 |
| **Impurity(ies)[#]** | Chloride | Cl | 0 - 0,5 | < 0,1 |
| | Water | $H_2O$ | 0 - 10 | < 5 |
| | Ammonium acetate | $C_2H_7NO_2$ | 0 – 8 | < 5 |
| | Several minor (especially metallic) impurities which do not affect the classification of the substance because of their non-hazardous nature or because they do not exceed the classification cut-off limits in the substance | e.g. Ag, Au, Cu, Ir, Pb, Pt, Rh, Ru | 0 - 0,5 | < 0,5 |

***** ≥ 80 % (w/w) for mono-constituent substances; ≥ 10 % (w/w) and < 80 % (w/w) for multi-constituent substances.

[#] An impurity is an unintended constituent present in a substance, as produced. It may originate from the starting materials or be the result of secondary or incomplete reactions during the production process. While impurities are present in the final substance, they were

not intentionally added.
§ Concentration ranges define the substance sameness criteria agreed by all Consortium Members in preparation of the communication with other SIEF members.
§§ Typical concentration refers to the representative sample used for testing.
$ Corresponds to 30-36.4 % Pd.

The composition given above is the composition of the solid substance. In practice, Tetraamminepalladium(2+) diacetate is only brought on the market in solution (usually with 15 – 20 % Pd content). The solvent can however be separated without affecting the chemical stability of the substance. The solid form is thus considered the same substance as the substance in solution; the solutions are considered mixtures under REACH.

## 6. Information on appearance, physical state and properties of the substance

**Table 5. Appearance / physical state / properties of the solid substance**

| | |
|---|---|
| **Physical state** | Solid |
| **Physical form*** | Crystalline |
| **Appearance** | White / Pale yellow crystals |
| **Particle size**** | Fine to coarse powder |
| **Does the solid hydrolyse?#** | No |
| **Is the solid hygroscopic?§** | Yes / No |

***** Crystalline form: solid material whose constituent atoms, molecules, or ions are arranged in an ordered pattern extending in all three spatial dimensions. Amorphous form: solid material whose constituent atoms, molecules, or ions are randomly arranged.
** Nanoform: particles in the size range 1 - 100 nm (for full definition of a nanomaterial, see http://ec.europa.eu/environment/chemicals/nanotech/index.htm#definition). Fine powder: particles in the size range 100 – 2.500 nm. Coarse powder: particles in the size range 2.500 nm – 1 mm. Massive object: particles in the size range > 1 mm.
# Hydrolysis: decomposition (cleavage of chemical bonds) by the addition of water.
§ Hygroscopic substance: readily attracts moisture from its surroundings in open air, through either absorption or adsorption. Cf. also water/moisture content in Table 4.

**Table 6. Appearance / physical state / properties of the substance in solution**

| | |
|---|---|
| **Physical state** | Solution |
| **Solvent** | Water |
| **Concentration range of substance in solution** | 41-55%$ |
| **pH (range) of the solution** | 7 - 9 |
| **Excess acid** | |

$ Corresponds to 15-20 % Pd.

## 7. Analytical data

Annex VI of REACH requires the registrant to describe the analytical methods and/or to provide the bibliographical references for the methods used for identification of the substance and, where appropriate, for the identification of impurities and additives. This information should be sufficient to allow the methods to be reproduced.

**Table 7. Analytical methods for identification of the substance**

| Parameter / Method | Recommended for substance identification and sameness check | Applicable | Not applicable or not recommended |
|---|---|---|---|
| **Elemental analysis** | | | |
| ICP (ICP-MS or ICP-OES) | X | | |
| Atomic absorption spectroscopy (AAS) | | | |
| Glow discharge mass spectrometry (GDMS) | | | |
| **Molecular analysis** | | | |
| Infrared (IR) spectroscopy | X (solid) | | |
| Raman spectroscopy | X (solution) | | |
| **Mineralogical analysis** | | | |
| X-Ray Fluorescence (XRF) | | X | |
| X-Ray Diffraction (XRD) | X | | |
| **Morphology and particle sizing** | | | |
| Electron microscopy (SEM, TEM, REM)* # | | | |
| Laser diffraction* # | X | | |
| Particle size by other means (e.g. sieve analysis)# | | | |
| Surface area by N-BET* # | X | | |
| **Other** | | | |
| | | | |

* Analytical techniques particularly (but not exclusively) relevant for nanomaterials.
# The choice of the technique for particle size depends on the size of the material as manufactured/imported/placed on the market/used.

## 8. Lead Registrant

Umicore AG & Co. KG (Germany) volunteers to be the Lead Registrant for Tetraamminepalladium(2+) diacetate. The EPMF will provide support to the Lead Registrant as laid down in the EPMF Agreement.

## 9. REACH Strategy

The table below presents the overall Registration Strategy for Tetraamminepalladium(2+) diacetate based on the information available to the EPMF by the date given above on the document.
The Registration Dossier will be prepared for the highest substance status (information requirements associated to a substance or Article 10 Registration being higher than an intermediate handled under strictly controlled conditions or Article 17 or 18 one) and associated tonnage band.
The recap below therefore reflects the scope of work of the EPMF for Tetraamminepalladium(2+) diacetate and sets the minimum and maximum set of information that will be gathered and/or produced when preparing the Registration Dossier for Tetraamminepalladium(2+) diacetate as described in this ID Card.
If higher information requirements are necessary, these can be included in the Registration dossier (if EPMF is made aware of these additional requirements in-time) as an update to the already submitted dossier.

**Table 8. REACH strategy for the substance (basis for REACH Registration preparation)**

| Item | Description |
|---|---|
| **REACH category** | Mono-constituent substance |
| **Highest status** | Substance |
| **Highest tonnage band** | 10 – 100 t/a |
| **Information requirements** | Available / Existing + Annex VII + Annex VIII |
| **Existing classification*** | Acute Tox. 4 (H302) (oral)<br>Skin Sens 1A (H317)<br>Eye Irr. 2 (H319)<br>Aquatic Acute 1 (H400)<br>Aquatic Chronic 1 (H410)<br>Acute M-factor 10<br>Chronic M-factor 10 |
| **Registration deadline** | 2018 |

***** For the pure form, as in the REACH registration dossier

## 10. Scope of the Registration Dossier

The uses included in this Registration Dossier are listed on the EPMF website.

## 11. Analytical reference information

Below the results of IR (solid) and Raman (solution) analysis of a reference sample.

**IR analysis solid form**
Spectrometer: Infrared spectrometer Tensor 27, BRUKER Optics
Spectral range: 4000 - 300 cm-1
Resolution: 2 cm-1
Scans: 32 scans
Temperature: ambient
Sample preparation: attenuated total reflection

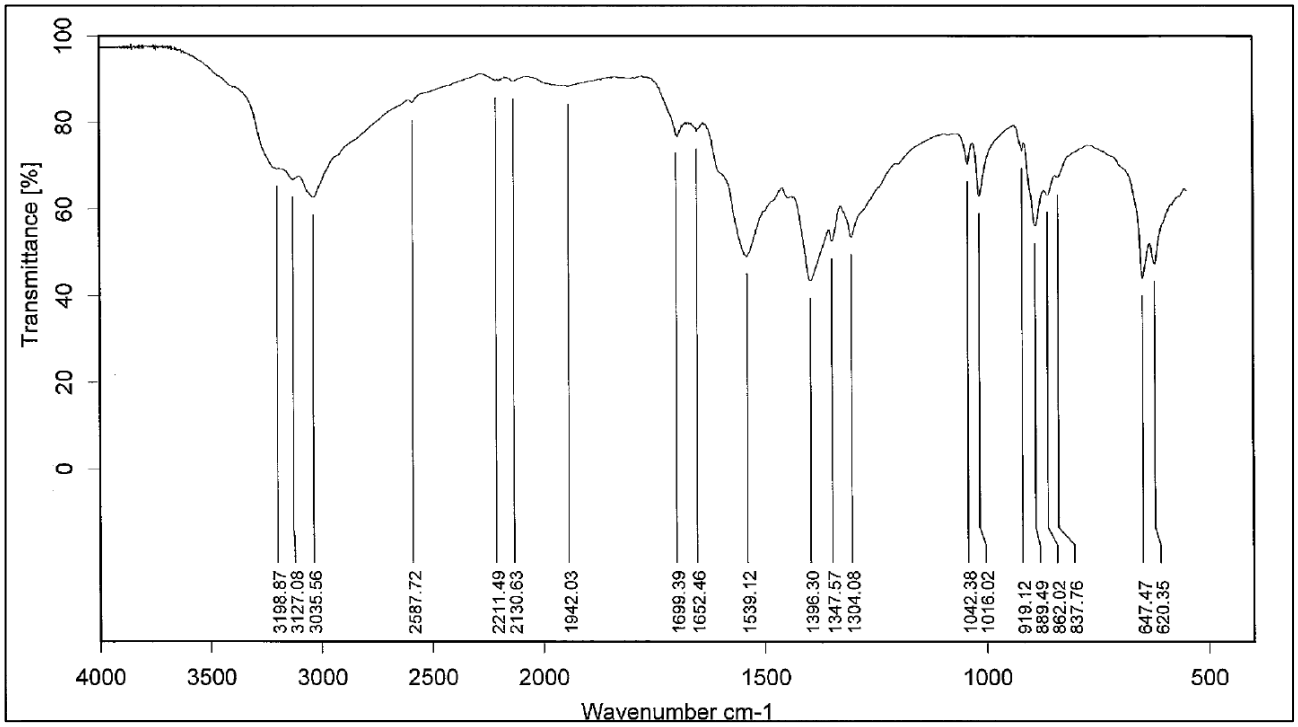



**Figure 1. IR spectrum of Tetraamminepalladium(2+) diacetate (solid)**

**Raman analysis solution**
Spectrometer: Bruker RFS 100/S
Spectral range: 3500 – 50 cm-1
Resolution: 2 cm-1
Scans: 100 scans
Laser: 1003 mW
Temperature: ambient
Sample preparation: liquid, glass vail

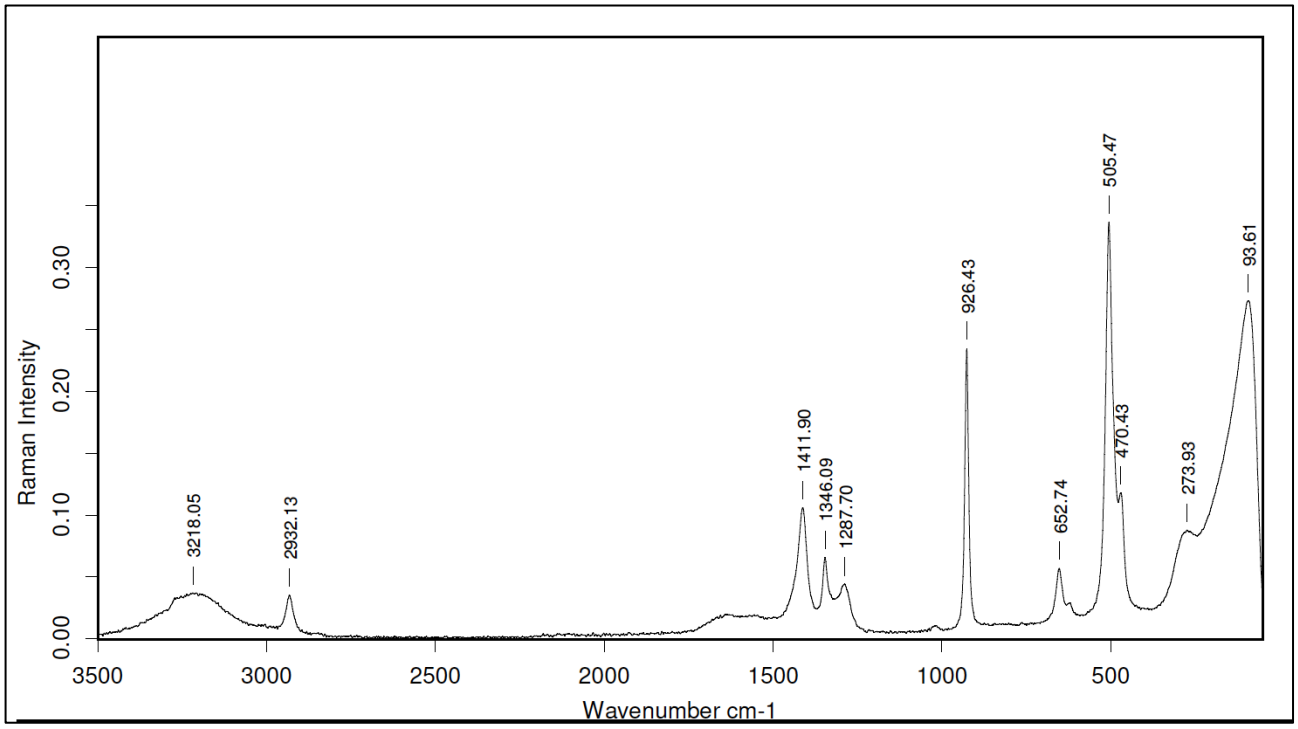



**Figure 2. Raman spectrum of Tetraamminepalladium(2+) diacetate (solution)**